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Author(s): J. Wendelberger
K. Campbell

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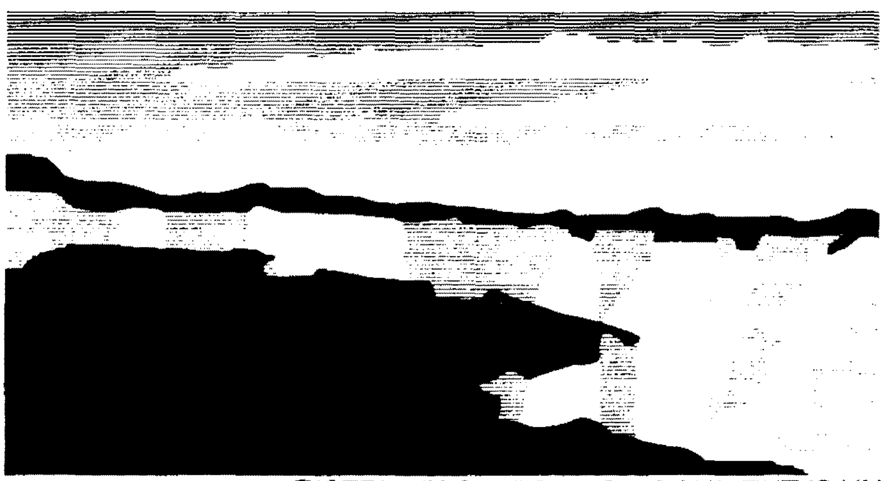

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NONDETECT DATA IN ENVIRONMENTAL INVESTIGATIONS

Joanne Wendelberger and Katherine Campbell, Los Alamos National Laboratory

Los Alamos National Laboratory, MS-F600, Los Alamos, NM 87545

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1. INTRODUCTION

Environmental data frequently contain values that are below detection limits. Values that are below detection limits are reported as being less than some reported limit of detection, rather than as actual values. Detection limits may vary for sample and reference datasets or even for individual observations. The implications of these nondetects in the summary, analysis, and interpretation of environmental data are explored. Alternative approaches for handling nondetect data are examined, with practical considerations being a key element in the selection of appropriate methodology.

Two general approaches may be used in the statistical analysis of data that contain nondetect values: 1) The nondetect values may be replaced using one of a variety of replacement methods, or 2) statistical techniques may be employed which can handle nondetect data. One of the most commonly used replacement methods is to substitute each nondetect value by half of its detection limit. Other commonly used replacement values are zeros or the detection limits. To avoid clumping of replaced values in cases where there are several nondetect values that share a common detection limit, values may be spaced evenly from 0 to the detection limit or according to some specified probability distribution.

This paper will review selected work that has been conducted on the handling of nondetects and examine specific environmental decisions in the presence of nondetect values.

2. NON-DETECT VALUES

Currie (1984, 1968) has noted that there are many different definitions of nondetect values in the scientific literature and has attempted to clarify the statistical error structure implied by the presence of nondetect values. Lambert, Peterson and Terpenning (1991) examined the nature of nondetects using extensive information on the actual measured values associated with nondetect values and showed that common reporting practices can throw out valuable information. In practice, the exact nature of the nondetect values may not be known. Information of the type used by Lambert et al may not be available. Instead, the statistician is left with the task of trying to make decisions in the situation where some of the values are only known to be less than specified values. In some cases, clear-cut decisions may be possible from the existing information. However, in border-line cases, additional values and additional information about the nature of the nondetect values may be worth obtaining to make better-informed decisions. Porter, Ward and Bell (1988) discuss the merits of having actual measured values rather than values recorded as nondetects.

In actual practice, the source of the chemical analysis measurements may be sufficiently far removed that the exact nature of the nondetect values is unknown. Instead, the analyst only knows that the measured value is less than or equal to the specified detection limit. EPA (1989, 1992a, 1992b) describes some of the different types of nondetect values that can occur with analytical data and makes some limited suggestions about the treatment of this type of data.

In the statistical literature, the term *censored data* is applied to data for which values above or below a certain threshold are not able to be measured. Cohen (1959) has proposed an approach for computing maximum likelihood estimators for the mean and variance of normally distributed data in the presence of censored values.

Several authors have examined censoring specifically in the context of environmental data. Gleit (1985) discusses estimation for small normal data sets with detection limits and compares several estimators via simulation. Hinton (1993) examines the performance of the delta log-normal method for estimating the mean of environmental data. This method assumes that the underlying distribution of values is a mixture of nonzero lognormal values and zeroes. Newman and Dixon (1990) describe a computer program with 5 different methods for estimating the mean and standard deviation from normal and lognormal data. Owen and DeRouen (1980) compare the robustness to deviations from model assumptions of two different methods for estimating the mean for lognormal data containing zeroes and left-censored values. Shumway, Azari and Johnson describe a method for estimating mean concentrations for environmental data with nondetects that uses transformations of the data. Travis and Land (1990) discuss the use of log-probit analysis to estimate the mean from a lognormal distribution with nondetects. Gillom (1984) looks at the effect of nondetects on the ability to detect trends.

In the following sections, specific environmental decisions will be considered where non-detects may need to be addressed.

3. DATA SUMMARY

Environmental investigations can result in the collection of large volumes of chemical analysis data. A single environmental sample may be divided up and analyzed for hundreds of different radiological or chemical constituents. Depending on the size of the site under investigation, the number of samples collected may range from less than 10 to several hundred.

An important step in the reporting and analysis of large quantities of data is to summarize the individual values. The presence of nondetect values can make summarization a non-trivial task, because common sample statistics such as the median, mean, standard deviation, maximum and minimum are not clearly defined for the case where nondetect values are present.

To convey meaningful information, the summary must either provide separate information for detect and nondetect data, follow a specified procedure for replacement of nondetects by proxy values prior to the computation of sample statistics, or must use statistical techniques to provide estimates of sample quantities based on the full dataset. Helsel (1990) and Helsel and Cohn (1988) discuss the estimation of descriptive statistics for data with nondetects.

How the data is intended to be used may help determine the most appropriate method of handling the nondetect values. As urged by EPA (1989), "Do not simply omit the nondetected results..." The authors have encountered cases where individuals have simply omitted all non-detects from a data summary. Clearly, this practice can seriously bias any summary statistics computed from the data. The method of handling nondetects may also depend on what type of constituent is being examined. When a number of closely related constituents are being considered, the replacement of nondetects may be achieved from a multiple constituent standpoint. For example, for polycyclic aromatic hydrocarbons (PAHs), one method that has been proposed is to set all nondetects to zero if there are no detected PAHs in a given sample and to set all nondetects to their corresponding detection limits if one or more of the PAHs are present above a detection limit.

4. COMPARISONS TO FIXED VALUES

In some cases, individual values or sample means must be compared to specified fixed levels to make a decision about whether further action is required at a site. At Los Alamos National Laboratory, a large number of sites are currently being investigated to determine whether contamination is present. In order to focus available resources on sites that require remediation, an initial screening is performed. Samples are collected at the sites and analyzed for a large number of constituents. The maximum values for each constituent are then compared to risk-based Screening Action Levels (SALs) to determine whether additional evaluation is required. In most cases, the detection limits are well below the SALs so nondetect values do not impact screening decisions. However, in some cases, the detection limits may be near the SALs or even above the SALs making comparisons difficult. When a simple comparison can not be made, alternative evaluation methods may be used. For example, historical knowledge of the site and the frequency of detected values in the dataset may be considered. Alternatively, comparisons to relevant background levels or risk assessment methodology, which are described in the next two sections, may be required.

5. COMPARING POPULATIONS

Non-detect values can pose an especially difficult problem when the goal is to compare two different populations. For example, data collected from an area suspected of possible contamination might be compared to data collected from some suitable background area that is similar, but known to be uncontaminated. Since the values sampled from the two populations may involve different censoring mechanisms and different limits of detection, care must be taken in order to arrive at valid conclusions. Gilbert and Simpson (1990, 1992) discuss several methods for comparing sample and reference populations and provide some advice on dealing with nondetects.

One simple approach is to apply standard parametric techniques with nondetects replaced by proxy values. A preferred approach may be to use nonparametric approaches. Hipel (1988) and Helsel (1987) discuss the advantages of using nonparametric techniques for the assessment of environmental data. Some nonparametric techniques can handle nondetect values directly. Others may require replacement of the nondetect values, but the exact values will have less impact than for parametric approaches. In other cases, the nonparametric techniques can handle nondetect values if certain assumptions may be made, such as all of the nondetect values being less than all of the values above detection limits.

The Wilcoxon test is a nonparametric test that may be used to compare samples from two populations. (See for example, Conover (1980).) The Wilcoxon test is effective for detecting location shifts of a distribution. The Wilcoxon test uses the ranks obtained from the dataset formed by combining the two samples. The test statistic is the sum of the ranks corresponding to one of the samples. For moderate to large sample sizes, a normal approximation may be used. Gehan (1965) proposed an extension of the Wilcoxon statistic for comparing two samples to handle censored data in the singly-censored case where all values are censored at the same value. Efron (1967) has proposed an alternative test statistic for the two sample problem with censored data.

When there are nondetects with multiple detection limits present, a multiple detection limit approach is required. Millard and Deverel (1988) discuss methods for comparing two sites when there are multiple detection limits and provide a comparison of various techniques based on a simulation study.

Another approach that may be especially appropriate for environmental applications is a quantile test developed by Johnson, Verrill and Moore (1987). This method examines the upper tail behavior of two populations by computing the probability that k out of the n largest values from the combined data set of $n_1 + n_2$ values would come from one of the populations if the two populations had the same distribution. This method will detect differences in the upper tail of the distribution. In environmental applications, it is often these extreme values which are of most interest. Since nondetect values tend to occur in the lower end of the distribution, this method can be used in the presence of nondetect data, provided the nondetect values are not among the n largest values. Even if some of the nondetect values are in the set of n largest values, the method could still be used if a replacement method was used to provide proxy values for the nondetects.

6. RISK ASSESSMENT

Risk assessment involves summarization of contaminant concentrations over areas called exposure units that represent physical area sizes encountered by individuals under a given land use scenario. The risk assessment process uses sample information about average contaminant concentrations to determine whether a particular area poses a human health risk. The 95% upper confidence limit on the mean is typically used as a reasonable maximum concentration for an exposed individual. (See EPA (1989).)

To examine the impact of nondetect values on risk assessment, consider the formula used in computing the 95% upper confidence limit on the mean. This formula involves not only the sample mean, but also the sample standard deviation. Replacement of nondetect values by their detection limits is generally regarded as conservative when estimating the mean because it will provide a mean estimate that is greater than or equal to the mean that would be obtained if the nondetect values were known. However, this replacement method will produce a smaller than desired standard deviation. The overall impact of replacing nondetects by their detection limits will depend on the relative magnitudes of the differences in the resulting mean and standard deviation from their true values induced by the replacement of the nondetects. If a simple replacement method is used, care should be taken that the resulting values do not result in an underestimate of the reasonable maximum values present at the site.

7. SUMMARY

Non-detect values are frequently encountered in the analysis of environmental data. The manner in which the nondetect values are handled should depend on the type of decision to be made and the magnitude and frequency of the nondetect values. If the nondetects are small in magnitude or low in frequency, the method of handling the nondetects will probably have minimal impact on the final outcome of the analysis. However, if the detection limits are close to important decision values, or if the frequency of nondetects is high, the treatment of the nondetect values can greatly influence resulting decisions.

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REFERENCES

1. Cohen, A. C. (1959), "Simplified Estimators for the Normal Distribution When Samples are Singly Censored or Truncated," *Technometrics*, 1, 3, 217-237.

3. Conover, W. J. (1980), *Practical Nonparametric Statistics*, 2nd Ed., John Wiley & Sons, New York.

4. Currie, L. A. (1984), *Lower Limit of Detection: Definition and Elaboration of a Proposed Position for Radiological Effluent and Environmental Measurements*, National Bureau of Standards, prepared for U. S. Nuclear Regulatory Commission, NUREG/CR-4007, Washington, DC.

5. Currie, L. A. (1968), ''Limits for Qualitative Detection and Quantitative Determination, Application to Radiochemistry," *Analytical Chemistry*, **40**, 3, 586-593.

6. Efron, B. (1967), ''The Two Sample Problem with Censored Data," Proceedings of the Fifth Berkeley Symposium, 831-853.

7. EPA (US Environmental Protection Agency) (1989), *Risk Assessment Guidance for Superfund, Volume I, Human Health Evaluation Manual (Part A)*, Interim Final, EPA540/1-89/002, Office of Emergency and Remedial Response, Washington, DC.

8. EPA (US Environmental Protection Agency) (1992a), *Guidance for Data Useability in Risk Assessment (Part A)*, Final, Publication 9285.7-09A, Office of Emergency and Remedial Response, Washington, DC.

9. EPA (US Environmental Protection Agency) (1992b), *Guidance for Data Useability in Risk Assessment (Part B)*, Final, Publication 9285.7-09B, Office of Emergency and Remedial Response, Washington, DC.

10. Gehan, E. A. (1965), ''A Generalized Wilcoxon Test for Comparing Arbitrarily Singly-Censored Samples," *Biometrika*, **52**, 203-223.

11. Gilbert, R. O. and Simpson, J. C. (1992), ''Statistical Methods for Evaluating the Attainment

of Cleanup Standards, Vol. 3: Reference-Based Standards for Soils and Solid Media," prepared for the U. S. Environmental Protection Agency, Pacific Northwest Laboratory, PNL-7409, Vol. 3, Rev. 1.

12. Gilbert, R. O. and Simpson, J. C. (1990), "Statistical Sampling and Analysis Issues and Needs for Testing Attainment of Background-Based Cleanup Standards at Superfund Sites," *Proceedings of the Workshop on Superfund Hazardous Waste: Statistical Issues in Characterizing a Site: Protocols, Tools, and Research Needs*, ed. by Lacayo et al, Center for Statistical Ecology and Environmental Statistics, University Park, PA.

13. Gillom, R. J., Hirsch, R. M. and Gilroy, E. J. (1984), "Effect of Censoring Trace-Level Water-Quality Data on Trend-Detection Capability," *Environ. Sci. Technol.*, **18**, 530-535.

14. Gleit, A. (1985), "Estimation for Small Normal Data Sets with Detection Limits," *Environ. Sci. Technol.*, **19**, 1201-1206.

15. Helsel, D. R. (1990), "Less than Obvious: Statistical Treatment of Data Below the Detection Limit," *Environ. Sci. Technol.*, **24**, 12, 1766-1774.

16. Helsel, D. R. (1987), "Advantages of Nonparametric Procedures for Analysis of Water Quality Data," *Hydrological Sciences*, **32**, 2, 179-190.

17. Helsel, D. R. and Cohn, T. A. (1988), "Estimation of Descriptive Statistics for Multiply Censored Water Quality Data," *Water Resources Research*, **24**, 12, 1997-2004.

18. Hinton, S. W. (1993), "Delta Log-Normal Statistical Methodology Performance," *Environ. Sci. Technol.*, **27**, 2247-2249.

19. Hipel, K. W. (1988), "Nonparametric Approaches to Environmental Impact Assessment," *Water Resources Bulletin*, **24**, 3, 487-492.

20. Johnson, R. A., Verrill, S. and Moore, D. H. (1987), ''Two-Sample Rank Tests for Detecting Changes That Occur in a Small Proportion of the Treated Population, *Biometrics*, **43**, 641-655.

21. Lambert, D., Peterson, B. and Terpenning, I. (1991), ''Nondetects, Detection Limits, and the Probability of Detection," *Journal of the American Statistical Association,*, **86**, 414, 266-277.

22. Millard, S. P. and Deverel, S. J. (1988), ''Nonparametric Statistical Methods for Comparing Two Sites Based on Data with Multiple Nondetect Limits," *Water Resources Research*, **24**, 12, 2087-2098.

23. Newman, M. C. and Dixon, P. M. (1990), ''UNCENSOR: A Program to Estimate Means and Standard Deviations for Data Sets with Below Detection Limit Observations," *American Environmental Laboratory*, **4**, 26-30.

24. Owen, W. J. and DeRouen, T. A. (1980), ''Estimation of the Mean for Lognormal Data Containing Zeroes and Left-Censored Values, with Applications to the Measurement of Worker Exposure to Air Contaminants," *Biometrics*, **36**, 707-719.

25. Porter, P. S., Ward, R. C. and Bell, H. F. (1988), ''The Detection Limit: Water Quality Monitoring Data are Plagued with Levels of Chemicals that Are Too Low to be Measured Precisely," *Environ. Sci. Technol.*, **22**, 8, 856-861.

26. Shumway, R. H., Azari, A. S. and Johnson, P. (1989), ''Estimating Mean Concentrations Under Transformation for Environmental Data with Detection Limits, *Technometrics*, **31**, 3, 347-356.

27. Travis, C. C. and Land, M. L. (1990), ''Estimating the Mean of Data Sets with Nondetectable

Values," *Environ. Sci. Technol.*, **24**, 7, 961-962.